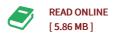




# **Ab Initio Molecular Dynamics**

By Marx, Dominik / Hutter, Jürg

Condition: New. Publisher/Verlag: Cambridge University Press | Basic Theory and Advanced Methods | The first book on this rapidly growing field for graduate students and researchers, covering a range of methods and applications. | Ab initio molecular dynamics revolutionized the field of realistic computer simulation of complex molecular systems and processes, including chemical reactions, by unifying molecular dynamics and electronic structure theory. This book provides the first coherent presentation of this rapidly growing field, covering a vast range of methods and their applications, from basic theory to advanced methods. This fascinating text for graduate students and researchers contains systematic derivations of various ab initio molecular dynamics techniques in order that readers can understand and assess the merits and drawbacks of commonly used methods. It also discusses the special features of the widely-used Car-Parrinello approach, correcting various misconceptions currently found in research literature. The book also contains pseudo-code and program layout for typical plane wave electronic structure codes, allowing newcomers to the field to understand commonly-used program packages, and enabling developers to improve and add new features in their code. | Part I. Basic Techniques: 1. Setting the stage: why ab initio molecular dynamics?; 2. Getting started: unifying Md and electronic...



# Reviews

Very beneficial to all of class of people. I am quite late in start reading this one, but better then never. You may like just how the writer create this publication.

-- Audra Klocko PhD

Thorough information! Its this type of great go through. It is amongst the most incredible publication i actually have read through. It is extremely difficult to leave it before concluding, once you begin to read the book.

-- Germaine Welch

## Related eBooks



#### Would It Kill You to Stop Doing

#### That?

Book Condition: New. Publisher/Verlag: Little, Brown Book Group | A Modern Guide to Manners | A laugh-out-loud guide to modern manners by acclaimed humorist, author, and Vanity Fair columnist Henry Alford. | A few years ago, humorist and journalist Henry Alford found



## Violet Rose and the Surprise

#### Party

Book Condition: New. Publisher/Verlag: Nosy Crow | With activities, 3D press-out models and over 175 stickers! Plus free games and printables online! | When busy rabbit, Violet Rose, discovers that her friend Lily has a birthday coming up, she and her buddies...



# Read Write Inc. Phonics: Orange Set 4 Storybook 2 I Think I Want to be a

#### 3ee

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 209 x 149 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read Write Inc. Set 1 and 2 sounds



# Study and Master English Grade 6 Core Reader: First Additional Language

Cambridge University Press (South Africa). Paperback. Book Condition: new. BRAND NEW, Study and Master English Grade 6 Core Reader: First Additional Language, Karen Morrison, Fiona Macgregor, Daphne Paizee, Study & Master English First Additional Language has been especially developed by an experienced...



# Read Write Inc. Phonics: Orange Set 4 Storybook 6 a Good

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. Tim Archbold (illustrator). 210 x 148 mm. Language: N/A. Brand New Book. These engaging Storybooks provide structured practice for children learning to read the Read Write Inc. Set 1 and 2 sounds....



## scientific literature retrieval practical tutorial (Chinese Edition)

paperback. Book Condition: New. Ship out in 2 business day, And Fast shipping, Free Tracking number will be provided after the shipment. Pages Number: 241 Publisher: Chongqing University Press Pub. Date: 2003-08. This book is the second edition of seven years after the...